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Oxidation and magnetic states of chalcopyrite CuFeS2: A first principles calculation

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Abstract

The ground state band structure, magnetic moments, charges and population numbers of electronic shells of Cu and Fe atoms have been calculated for chalcopyrite CuFeS2 using density functional theory. The comparison between our calculation results and experimental data (X-ray photoemission, X-ray absorption and neutron diffraction spectroscopy) has been made. Our calculations predict a formal oxidation state for chalcopyrite as Cu 1+Fe3+S2 2-. However, the assignment of formal valence state to transition metal atoms appears to be oversimplified. It is anticipated that the valence state can be confirmed experimentally by nuclear magnetic and nuclear quadrupole resonance and Mössbauer spectroscopy methods. © 2014 Pleiades Publishing, Ltd.

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